

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $1.31\text{e-}11$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $8.36\text{e-}01$

**Confidence level:**  $9.11\text{e-}01$

## Nearest Neighbors from the Training Set

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Dodecane

**Measured:**  $1.42\text{e-}11$

**Predicted:**  $1.31\text{e-}11$

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Tridecane

**Measured:**  $1.60\text{e-}11$

**Predicted:**  $1.64\text{e-}11$

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Undecane

**Measured:**  $1.32\text{e-}11$

**Predicted:**  $1.05\text{e-}11$

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4-Methyloctane

**Measured:**  $9.72\text{e-}12$

**Predicted:**  $9.18\text{e-}12$

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2-Methyloctane

**Measured:**  $1.01\text{e-}11$

**Predicted:**  $9.18\text{e-}12$